Louisiana Tech University Researchers Successfully Predict Mechanical Behavior of a Metal/Ceramic System with Validated Computational Approach

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What is the outcome or accomplishment? (1-2 short sentences describing it and why it is transformative; 50 word max. suggested)*

Louisiana Tech University (LATech) researchers applied a computational approach previously validated against experimental results to predict the behavior of a metal/ceramic interface that has not yet been subjected to experimental investigations.

What is the impact? (1-2 simple sentences describing the benefits for science, industry, society, the economy, national security, *etc.*; suggested 50 word maximum)

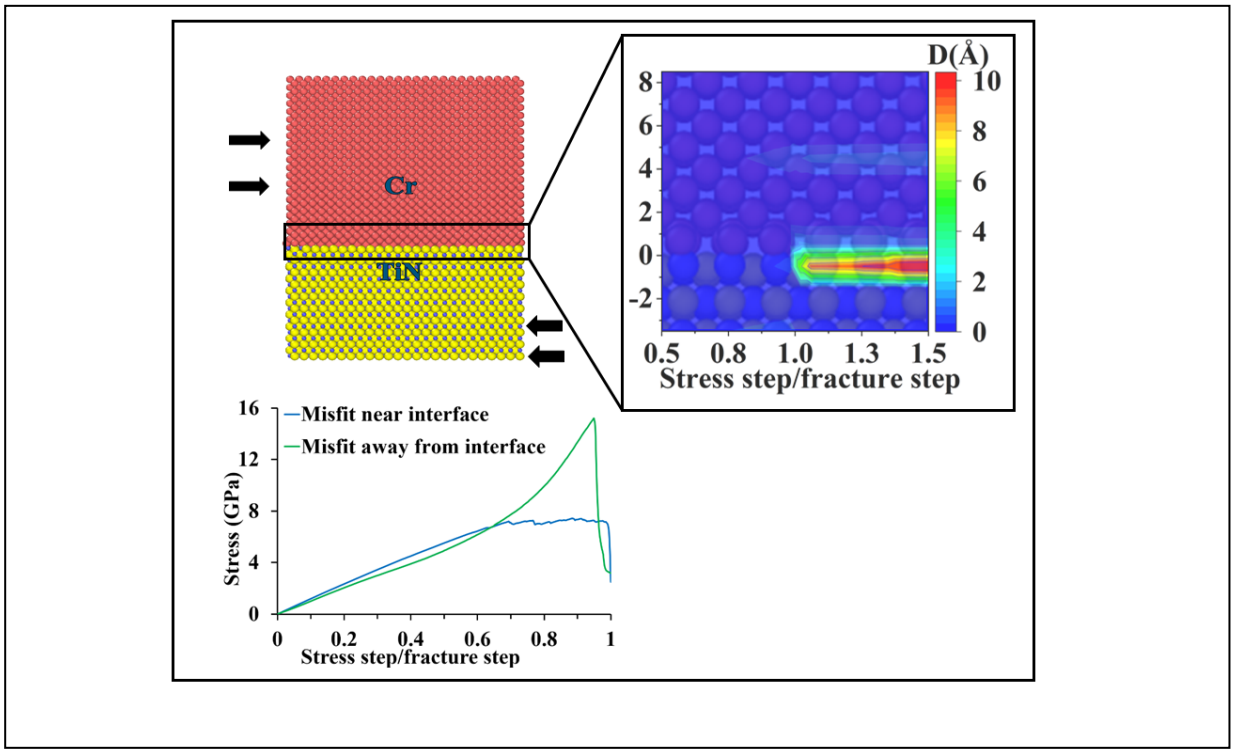
Experimentally validated simulations for metal/ceramic interfaces are useful to for designing such systems, and greatly reduce expensive laboratory trial-and-error and development time, and allow researchers to focus efforts on the most promising candidates.

What explanation/background does the lay reader need to understand the significance of this outcome? (1-2 paragraphs that might include, for example, more on who, when, where; NSF's role; support from multiple directorates/offices; what makes this accomplishment unique; additional intellectual merits; or broader impacts such as education, outreach, or infrastructure improvement that are integral to this outcome; suggested 150 word maximum)

The LATech team applied their simulation methods to study the Cr/TiN interface, which—to the best of their knowledge—represents the first bcc metal/NaCl type ceramic system to be subjected to such a computational study. The approach starts with first principles computations on a relatively small number of atoms. The results are then used to develop models for studies on larger systems containing many more atoms, and to investigate realistic systems.

From previous studies, which were validated against experimental results, the researchers identified properties from the first principles studies that reliably predict interfacial properties on a larger scale. In the case of Cr/TiN, the first principles simulations predicted that this system is able to resist shear deformation more effectively than previously studied metal/ceramic interfaces. It also predicted that the interfacial failure, when it occurs, is likely to be in the ceramic phase, which is also a novelty compared to previously examined systems.

The LATech researchers then developed the model for larger scale studies on the Cr/TiN system which are more appropriate for comparison to experimental results when they become available. This model allowed them to study the properties of the interface in relation to the so-called misfit dislocation networks which are manifested only at the larger scale. These simulations confirmed the conclusions drawn from the first principles studies that the interfacial failure occurs within the ceramic phase, away from the chemical interface separating Cr from TiN. The ability of this interface to withstand shear loading is attributed to the strong interaction between the nitrogen atoms in TiN with the Cr atoms in the metal phase.



This illustration shows the approach used to study the Cr/TiN interface. The results of first principles simulations on a small system are used to develop a model to study the interface at significantly larger length scales. These studies predict that the Cr/TiN system is very good at resisting stress due to shear deformation. It was also found that interfacial failure occurs away from the chemical interface, within the ceramic layers. Illustration by Nisha Dhariwal, Bala Ramachandran, and Collin D. Wick, Louisiana Tech University.